EXHIBIT D

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Amino acid residue environments and predictions of residue ty

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The determination of a protein's structure from the knowledge of its linear chain is one of the important problems that remains as a bottleneck in interpreting the rapidly increasing repository of genetic sequence data. One approach to this problem that has shown promise and given a measure of success is threading. In this approach contact energies between different ami acids are first determined by statistical methods applied to known structures. These contact energies are then applied to a sequence whose structure is to b determined by threading it through various known structures and determinin the total threading energy for each candidate structure. That structure that yields the lowest total energy is then considered the leading candidate amon all the structures tested. Additional information is often needed in order to support the results of threading studies, as it is well known in the field that t contact potentials used are not sufficiently sensitive to allow definitive conclusions. Here, we investigate the hypothesis that the environment of an amino acid residue realized as all those residues not local to it on the chain b sufficiently close spatially can supply information predictive of the type of t residue that is not adequately reflected in the individual contact energies. W present evidence that confirms this hypothesis and suggests a high order cooperativity between the residues that surround a given residue and how th interact with it. We suggest a possible application to threading.

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